Structure and stability of BaTiSi2O7 - DTU Orbit (13/10/2019)

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Due to their optical, photo-luminescence (PL), and afterglow properties, barium titanosilicates are compounds of great interest for functional materials and light-emitting devices. Among them, BaTiSi2O7 (BTS2) is certainly one of the most intriguing; it displays peculiar properties (e.g. PL orange emission) whose exhaustive explanation has been hampered to date by the lack of a structure model. In this work, BTS2 and the related compound BaTiSi4O11 (BTS4) were synthesized through conventional solid-state reaction methods. BTS2 invariably shows complex twinning patterns. Thus, its structure solution and Rietveld structure refinement were attempted using synchrotron powder diffraction. BTS2 was found to be an intergrowth of monoclinic and triclinic crystals. The monoclinic phase has the space group $P2_1/n$ and unit cell $a = 7.9836$ (3), $b = 10.0084$ (4), $c = 7.4795$ (3) Å, and $\beta = 100.321$ (3)$^\circ$, whereas the triclinic phase has the space group and unit cell $a = 7.99385$ (4), $b = 10.01017$ (5), $c = 7.47514$ (3) Å, $a = 90.084$ (8), $b = 100.368$ (8) and $c = 89.937$ (9)$^\circ$. These lattices can be seen as a distortion of that of tetragonal synthetic $\beta$-BaVSi2O7 with Ti in place of V. The structure models obtained from this study confirm the presence of fivefold coordinated Ti atoms in a distorted pyramidal configuration. The proposed solution supports existing theories for the explanation of the PL orange colour in BTS2.

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